



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:18 AM UTC

PDB ID : 9E22 / pdb\_00009e22  
EMDB ID : EMD-47429  
Title : Cryo-EM structure of human cytoplasmic dynein-1 bound to LIS1 in the presence of ATP  
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.  
Deposited on : 2024-10-21  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

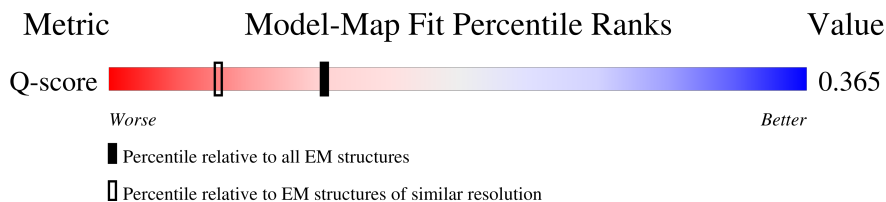
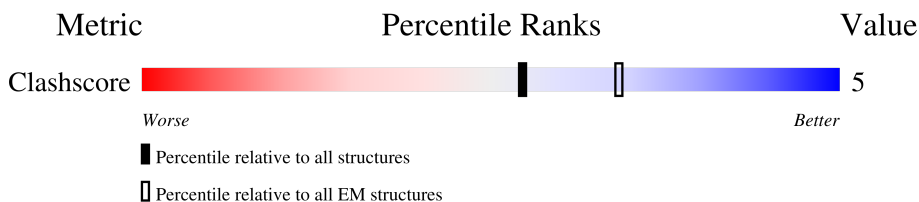
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

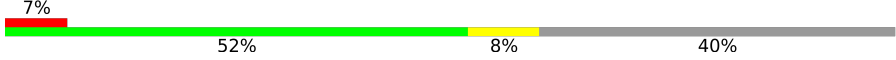

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	15087 ( 2.80 - 3.80 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4843	
2	E	411	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24612 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2925	Total	C	N	O	S	0	0
			22914	14535	3984	4283	112		

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-196	GLY	-	expression tag	UNP Q14204
A	-195	ASP	-	expression tag	UNP Q14204
A	-194	TYR	-	expression tag	UNP Q14204
A	-193	ASP	-	expression tag	UNP Q14204
A	-192	ILE	-	expression tag	UNP Q14204
A	-191	PRO	-	expression tag	UNP Q14204
A	-190	THR	-	expression tag	UNP Q14204
A	-189	THR	-	expression tag	UNP Q14204
A	-188	GLU	-	expression tag	UNP Q14204
A	-187	ASN	-	expression tag	UNP Q14204
A	-186	LEU	-	expression tag	UNP Q14204
A	-185	TYR	-	expression tag	UNP Q14204
A	-184	PHE	-	expression tag	UNP Q14204
A	-183	GLN	-	expression tag	UNP Q14204
A	-182	GLY	-	expression tag	UNP Q14204
A	-181	ASP	-	expression tag	UNP Q14204
A	-180	LYS	-	expression tag	UNP Q14204
A	-179	ASP	-	expression tag	UNP Q14204
A	-178	CYS	-	expression tag	UNP Q14204
A	-177	GLU	-	expression tag	UNP Q14204
A	-176	MET	-	expression tag	UNP Q14204
A	-175	LYS	-	expression tag	UNP Q14204
A	-174	ARG	-	expression tag	UNP Q14204
A	-173	THR	-	expression tag	UNP Q14204
A	-172	THR	-	expression tag	UNP Q14204
A	-171	LEU	-	expression tag	UNP Q14204
A	-170	ASP	-	expression tag	UNP Q14204
A	-169	SER	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-168	PRO	-	expression tag	UNP Q14204
A	-167	LEU	-	expression tag	UNP Q14204
A	-166	GLY	-	expression tag	UNP Q14204
A	-165	LYS	-	expression tag	UNP Q14204
A	-164	LEU	-	expression tag	UNP Q14204
A	-163	GLU	-	expression tag	UNP Q14204
A	-162	LEU	-	expression tag	UNP Q14204
A	-161	SER	-	expression tag	UNP Q14204
A	-160	GLY	-	expression tag	UNP Q14204
A	-159	CYS	-	expression tag	UNP Q14204
A	-158	GLU	-	expression tag	UNP Q14204
A	-157	GLN	-	expression tag	UNP Q14204
A	-156	GLY	-	expression tag	UNP Q14204
A	-155	LEU	-	expression tag	UNP Q14204
A	-154	HIS	-	expression tag	UNP Q14204
A	-153	ARG	-	expression tag	UNP Q14204
A	-152	ILE	-	expression tag	UNP Q14204
A	-151	ILE	-	expression tag	UNP Q14204
A	-150	PHE	-	expression tag	UNP Q14204
A	-149	LEU	-	expression tag	UNP Q14204
A	-148	GLY	-	expression tag	UNP Q14204
A	-147	LYS	-	expression tag	UNP Q14204
A	-146	GLY	-	expression tag	UNP Q14204
A	-145	THR	-	expression tag	UNP Q14204
A	-144	SER	-	expression tag	UNP Q14204
A	-143	ALA	-	expression tag	UNP Q14204
A	-142	ALA	-	expression tag	UNP Q14204
A	-141	ASP	-	expression tag	UNP Q14204
A	-140	ALA	-	expression tag	UNP Q14204
A	-139	VAL	-	expression tag	UNP Q14204
A	-138	GLU	-	expression tag	UNP Q14204
A	-137	VAL	-	expression tag	UNP Q14204
A	-136	PRO	-	expression tag	UNP Q14204
A	-135	ALA	-	expression tag	UNP Q14204
A	-134	PRO	-	expression tag	UNP Q14204
A	-133	ALA	-	expression tag	UNP Q14204
A	-132	ALA	-	expression tag	UNP Q14204
A	-131	VAL	-	expression tag	UNP Q14204
A	-130	LEU	-	expression tag	UNP Q14204
A	-129	GLY	-	expression tag	UNP Q14204
A	-128	GLY	-	expression tag	UNP Q14204
A	-127	PRO	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-126	GLU	-	expression tag	UNP Q14204
A	-125	PRO	-	expression tag	UNP Q14204
A	-124	LEU	-	expression tag	UNP Q14204
A	-123	MET	-	expression tag	UNP Q14204
A	-122	GLN	-	expression tag	UNP Q14204
A	-121	ALA	-	expression tag	UNP Q14204
A	-120	THR	-	expression tag	UNP Q14204
A	-119	ALA	-	expression tag	UNP Q14204
A	-118	TRP	-	expression tag	UNP Q14204
A	-117	LEU	-	expression tag	UNP Q14204
A	-116	ASN	-	expression tag	UNP Q14204
A	-115	ALA	-	expression tag	UNP Q14204
A	-114	TYR	-	expression tag	UNP Q14204
A	-113	PHE	-	expression tag	UNP Q14204
A	-112	HIS	-	expression tag	UNP Q14204
A	-111	GLN	-	expression tag	UNP Q14204
A	-110	PRO	-	expression tag	UNP Q14204
A	-109	GLU	-	expression tag	UNP Q14204
A	-108	ALA	-	expression tag	UNP Q14204
A	-107	ILE	-	expression tag	UNP Q14204
A	-106	GLU	-	expression tag	UNP Q14204
A	-105	GLU	-	expression tag	UNP Q14204
A	-104	PHE	-	expression tag	UNP Q14204
A	-103	PRO	-	expression tag	UNP Q14204
A	-102	VAL	-	expression tag	UNP Q14204
A	-101	PRO	-	expression tag	UNP Q14204
A	-100	ALA	-	expression tag	UNP Q14204
A	-99	LEU	-	expression tag	UNP Q14204
A	-98	HIS	-	expression tag	UNP Q14204
A	-97	HIS	-	expression tag	UNP Q14204
A	-96	PRO	-	expression tag	UNP Q14204
A	-95	VAL	-	expression tag	UNP Q14204
A	-94	PHE	-	expression tag	UNP Q14204
A	-93	GLN	-	expression tag	UNP Q14204
A	-92	GLN	-	expression tag	UNP Q14204
A	-91	GLU	-	expression tag	UNP Q14204
A	-90	SER	-	expression tag	UNP Q14204
A	-89	PHE	-	expression tag	UNP Q14204
A	-88	THR	-	expression tag	UNP Q14204
A	-87	ARG	-	expression tag	UNP Q14204
A	-86	GLN	-	expression tag	UNP Q14204
A	-85	VAL	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-84	LEU	-	expression tag	UNP Q14204
A	-83	TRP	-	expression tag	UNP Q14204
A	-82	LYS	-	expression tag	UNP Q14204
A	-81	LEU	-	expression tag	UNP Q14204
A	-80	LEU	-	expression tag	UNP Q14204
A	-79	LYS	-	expression tag	UNP Q14204
A	-78	VAL	-	expression tag	UNP Q14204
A	-77	VAL	-	expression tag	UNP Q14204
A	-76	LYS	-	expression tag	UNP Q14204
A	-75	PHE	-	expression tag	UNP Q14204
A	-74	GLY	-	expression tag	UNP Q14204
A	-73	GLU	-	expression tag	UNP Q14204
A	-72	VAL	-	expression tag	UNP Q14204
A	-71	ILE	-	expression tag	UNP Q14204
A	-70	SER	-	expression tag	UNP Q14204
A	-69	TYR	-	expression tag	UNP Q14204
A	-68	SER	-	expression tag	UNP Q14204
A	-67	HIS	-	expression tag	UNP Q14204
A	-66	LEU	-	expression tag	UNP Q14204
A	-65	ALA	-	expression tag	UNP Q14204
A	-64	ALA	-	expression tag	UNP Q14204
A	-63	LEU	-	expression tag	UNP Q14204
A	-62	ALA	-	expression tag	UNP Q14204
A	-61	GLY	-	expression tag	UNP Q14204
A	-60	ASN	-	expression tag	UNP Q14204
A	-59	PRO	-	expression tag	UNP Q14204
A	-58	ALA	-	expression tag	UNP Q14204
A	-57	ALA	-	expression tag	UNP Q14204
A	-56	THR	-	expression tag	UNP Q14204
A	-55	ALA	-	expression tag	UNP Q14204
A	-54	ALA	-	expression tag	UNP Q14204
A	-53	VAL	-	expression tag	UNP Q14204
A	-52	LYS	-	expression tag	UNP Q14204
A	-51	THR	-	expression tag	UNP Q14204
A	-50	ALA	-	expression tag	UNP Q14204
A	-49	LEU	-	expression tag	UNP Q14204
A	-48	SER	-	expression tag	UNP Q14204
A	-47	GLY	-	expression tag	UNP Q14204
A	-46	ASN	-	expression tag	UNP Q14204
A	-45	PRO	-	expression tag	UNP Q14204
A	-44	VAL	-	expression tag	UNP Q14204
A	-43	PRO	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	ILE	-	expression tag	UNP Q14204
A	-41	LEU	-	expression tag	UNP Q14204
A	-40	ILE	-	expression tag	UNP Q14204
A	-39	PRO	-	expression tag	UNP Q14204
A	-38	CYS	-	expression tag	UNP Q14204
A	-37	HIS	-	expression tag	UNP Q14204
A	-36	ARG	-	expression tag	UNP Q14204
A	-35	VAL	-	expression tag	UNP Q14204
A	-34	VAL	-	expression tag	UNP Q14204
A	-33	GLN	-	expression tag	UNP Q14204
A	-32	GLY	-	expression tag	UNP Q14204
A	-31	ASP	-	expression tag	UNP Q14204
A	-30	LEU	-	expression tag	UNP Q14204
A	-29	ASP	-	expression tag	UNP Q14204
A	-28	VAL	-	expression tag	UNP Q14204
A	-27	GLY	-	expression tag	UNP Q14204
A	-26	GLY	-	expression tag	UNP Q14204
A	-25	TYR	-	expression tag	UNP Q14204
A	-24	GLU	-	expression tag	UNP Q14204
A	-23	GLY	-	expression tag	UNP Q14204
A	-22	GLY	-	expression tag	UNP Q14204
A	-21	LEU	-	expression tag	UNP Q14204
A	-20	ALA	-	expression tag	UNP Q14204
A	-19	VAL	-	expression tag	UNP Q14204
A	-18	LYS	-	expression tag	UNP Q14204
A	-17	GLU	-	expression tag	UNP Q14204
A	-16	TRP	-	expression tag	UNP Q14204
A	-15	LEU	-	expression tag	UNP Q14204
A	-14	LEU	-	expression tag	UNP Q14204
A	-13	ALA	-	expression tag	UNP Q14204
A	-12	HIS	-	expression tag	UNP Q14204
A	-11	GLU	-	expression tag	UNP Q14204
A	-10	GLY	-	expression tag	UNP Q14204
A	-9	HIS	-	expression tag	UNP Q14204
A	-8	ARG	-	expression tag	UNP Q14204
A	-7	LEU	-	expression tag	UNP Q14204
A	-6	GLY	-	expression tag	UNP Q14204
A	-5	LYS	-	expression tag	UNP Q14204
A	-4	PRO	-	expression tag	UNP Q14204
A	-3	GLY	-	expression tag	UNP Q14204
A	-2	LEU	-	expression tag	UNP Q14204
A	-1	GLY	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q14204
A	1	SER	-	expression tag	UNP Q14204

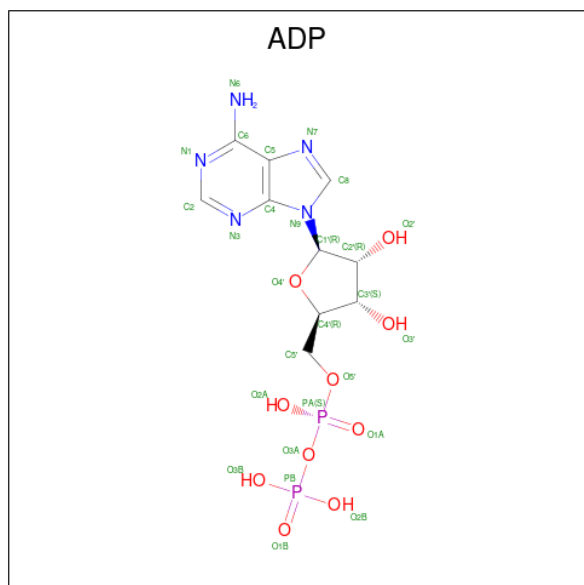
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	320	Total	C	N	O	0	0
			1581	940	320	321		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P43034
E	1	SER	-	expression tag	UNP P43034

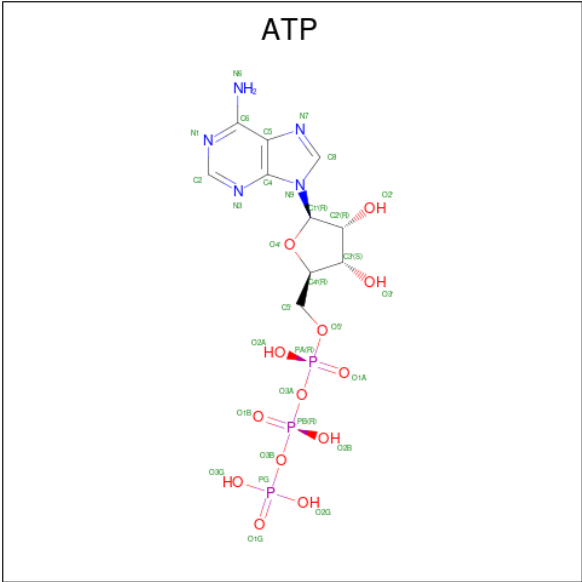
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

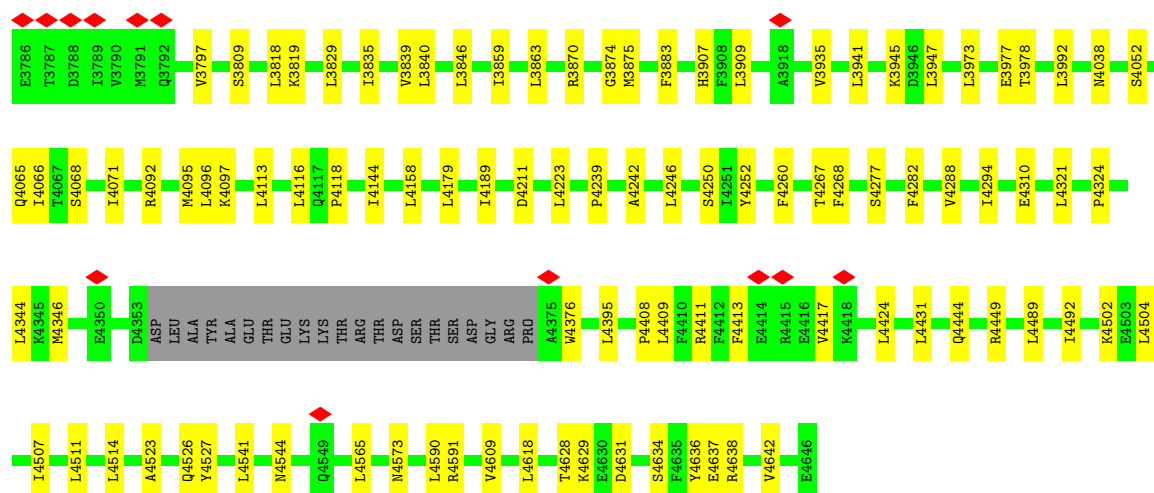
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

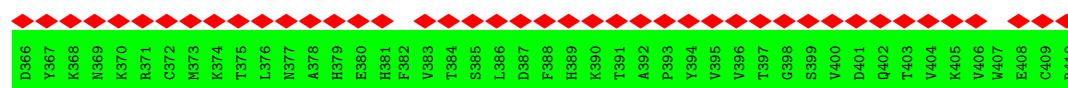
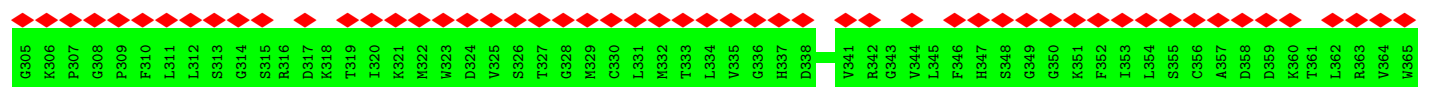
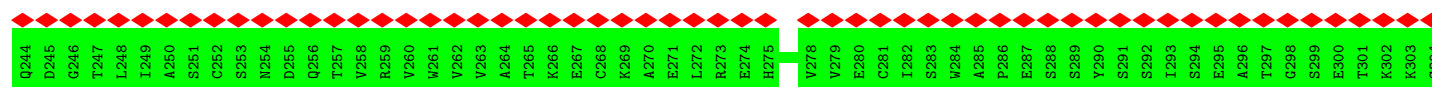
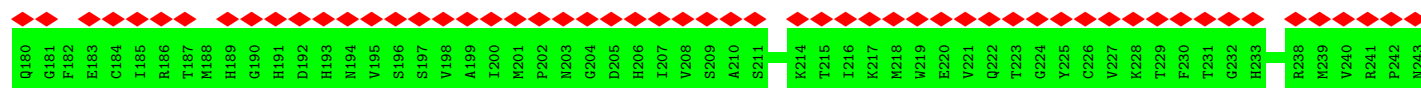
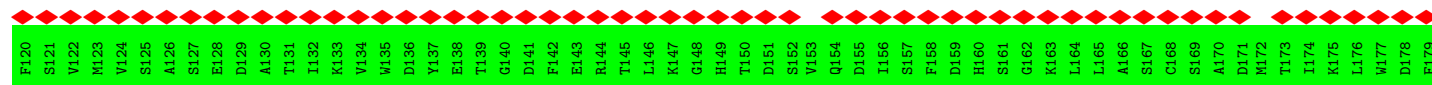
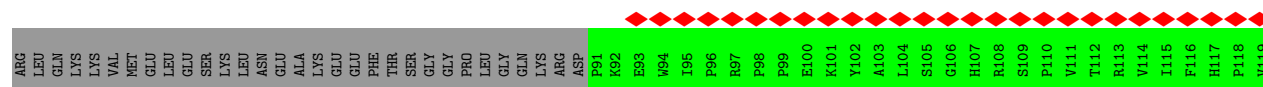
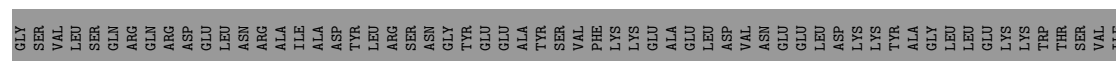
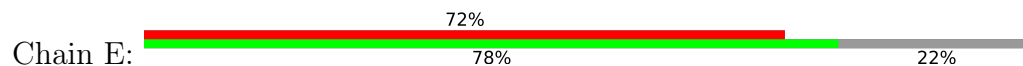


L1812	Q1612	Y1545	TRP	ASP	LEU	VAL	GLU	GLY	HIS	TYR	GLN	VAL	GLN	ALA	TRP	ILE	ARG	VAL
T1813	K1613	Y1546	VAL	ALA	GLU	GLN	GLU	GLN	GLY	VAL	GLN	VAL	GLU	ASP	GLU	VAL	LYS	SER
E1814	L1547	L1547	SER	LEU	THR	THR	ASP	VAL	VAL	GLY	VAL	VAL	ASP	GLY	SER	ASN	GLN	GLY
Q1818	E1548	E1548	GLU	ASN	THR	THR	ARG	GLU	LEU	VAL	ILE	LEU	LEU	LEU	LYS	HIS	ILE	ILE
F1836	G1549	G1549	LEU	GLN	GLY	GLY	VAL	TYR	TYR	TYR	LYS	TYR	GLY	ASN	ASP	GLN	TRP	ALA
L1839	I1550	I1550	THR	LEU	LEU	LEU	GLJ	ARG	GLY	GLU	GLY	GLU	GLY	HIS	PRO	ALA	LEU	ALA
F1551	G1488	R1488	THR	LEU	LEU	LEU	VAL	TYR	TYR	TYR	GLY	GLY	GLY	GLY	GLY	ALA	LEU	LEU
T1552	G1489	G1489	LEU	LYS	LEU	LEU	GLJ	ARG	ARG	GLU	ARG	ARG	GLY	ASN	TYR	GLN	GLY	LYS
G1553	W1490	W1490	GLY	PHE	SER	SER	ARG	GLY	GLY	THR	GLY	GLY	GLY	PRO	VAL	VAL	VAL	VAL
S1554	D1491	D1491	ILE	ASN	GLY	GLY	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SER	ILE
K1558	L1492	L1492	TRP	ALA	SER	SER	THR	ASP	GLY	GLU	GLY	LEU	ASP	ASN	ARG	TYR	GLY	ASP
H1559	L1493	L1493	ASP	LEU	GLU	GLU	LEU	LEU	LEU	LYS	SER	SER	LEU	ASN	PRO	PHE	ILE	ARG
I1560	F1494	F1494	VAL	LEU	ARG	ARG	LEU	LEU	GLU	LYS	GLY	GLY	GLY	ASN	ALA	ALA	GLN	GLN
L1560	N1495	N1495	THR	GLN	THR	THR	THR	THR	VAL	THR	VAL	VAL	VAL	VAL	THR	THR	PHE	THR
L1561	L1496	L1496	GLN	TYR	GLN	GLN	ASP	GLN	THR	GLN	THR	THR	THR	GLN	GLN	GLN	ILE	ALA
P1562	V1497	V1497	ASN	ALA	VAL	VAL	GLU	GLU	GLY	GLY	GLY	GLY	GLY	ASN	ASN	ASN	GLY	VAL
V1563	K1498	K1498	GLU	SER	ALA	ALA	GLU	GLU	PHE	GLN	PHE	GLY	GLY	LEU	LEU	LEU	THR	THR
Q1566	E1499	E1499	GLU	TYR	LEU	LEU	LYS	GLY	GLN	LYS	GLY	GLY	GLY	LEU	LEU	LEU	GLY	GLY
R1567	H1500	H1500	ALA	GLY	GLU	GLU	THR	THR	PHE	THR	SER	SER	SER	THR	THR	THR	THR	THR
F1568	I1501	I1501	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
S1570	V1504	V1504	ASP	LEU	ASP	ASP	GLY	GLY	ASP	THR	LYS	LYS	LYS	VAL	VAL	VAL	VAL	VAL
I1571	S1505	S1505	LEU	LEU	LYS	LYS	ASN	ASN	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S1572	A1506	A1506	GLY	GLY	VAL	VAL	VAL	VAL	GLY	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
T1573	W1507	W1507	THR	MET	THR	THR	GLU	GLU	THR	TRP	THR	THR	THR	THR	THR	THR	THR	THR
E1574	K1508	K1508	LYS	ILE	LEU	LEU	GLU	GLU	GLY	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
F1575	L1509	L1509	ILE	ASN	LEU	LEU	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1576	P1511	P1511	ASN	SER	SER	SER	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
A1577	Y1512	Y1512	LEU	VAL	VAL	VAL	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1578	K1513	K1513	VAL	THR	THR	THR	GLY	GLY	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR
M1579	L1514	L1514	ILE	ILE	GLU	GLU	THR	PHE	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
K1580	V1515	V1515	GLU	GLY	GLN	GLN	ILE	ASN	ASN	GLY	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
K1581	F1516	F1516	LYS	SER	GLN	GLN	GLY	MET	ARG	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
V1582	E1517	E1517	GLU	GLY	MET	LYS	PHE	ARG	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
S1583	D1519	D1519	LEU	ALA	GLU	GLU	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
K1584	A1520	A1520	LYS	LEU	GLN	GLN	ARG	ARG	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR
S1585	L1521	L1521	ASP	ASP	PRO	PRO	LEU	LEU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
P1586	S1522	S1522	HIS	TRP	VAL	VAL	ASP	ASP	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR
L1587	W1523	W1523	LYS	TRP	SER	SER	ASP	ASP	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
V1588	E1524	E1524	VAL	VAL	GLN	GLN	ARG	ARG	GLY	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR
M1589	D1525	D1525	GLN	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
D1590	K1526	K1526	LEU	LEU	PRO	PRO	CYS	CYS	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
V1591	L1527	L1527	LYS	ARG	LYS	LYS	ALA	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1592	N1528	N1528	THR	ARG	LEU	LEU	LYS	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
N1593	R1529	R1529	ILE	LEU	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
I1594	I1530	I1530	GLY	HIS	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q1595	M1531	M1531	VAL	VAL	ASN	ASN	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
G1596	A1532	A1532	ASP	ASP	VAL	VAL	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
V1597	L1533	L1533	LYS	LYS	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q1598	F1534	F1534	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
R1599	D1535	D1535	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S1600	V1536	V1536	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
L1601	W1537	W1537	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
E1602	I1538	I1538	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
R1603	D1539	D1539	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1604	V1540	V1540	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
A1605	Q1541	Q1541	ASP	ASP	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
D1606	R1542	R1542	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1607	W1544	W1544	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE





• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	610	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.918	Depositor
Minimum map value	-0.525	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.084	Depositor
Map size (Å)	329.12, 329.12, 329.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.14	0/23382	0.34	0/31728
2	E	0.08	0/1580	0.25	0/2197
All	All	0.14	0/24962	0.34	0/33925

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22914	0	22417	244	0
2	E	1581	0	693	0	0
3	A	54	0	24	1	0
4	A	62	0	24	0	0
5	A	1	0	0	0	0
All	All	24612	0	23158	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:ARG:O	1:A:3725:ASP:HB2	1.74	0.88
1:A:2231:SER:HB3	1:A:2344:GLU:OE2	1.78	0.83
1:A:3645:LEU:O	1:A:3649:LEU:HB2	1.81	0.80
1:A:3624:GLU:O	1:A:3628:ARG:HB2	1.84	0.77
1:A:2601:LYS:HB3	1:A:2736:VAL:HG21	1.70	0.72
1:A:1792:LEU:HD11	1:A:1808:LEU:HD22	1.72	0.72
1:A:1713:LEU:HD11	1:A:1870:PHE:HB3	1.75	0.68
1:A:2503:SER:HB3	1:A:2514:LEU:HD23	1.78	0.66
1:A:1640:ILE:HG12	1:A:1650:LEU:HG	1.78	0.66
1:A:3586:TYR:HD2	1:A:3649:LEU:HD12	1.62	0.64
1:A:3607:ARG:HB3	1:A:3632:PRO:HD3	1.79	0.64
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.80	0.64
1:A:1627:PRO:HB2	1:A:1951:VAL:HB	1.79	0.64
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.79	0.64
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.80	0.63
1:A:1622:GLU:HA	1:A:1699:ASN:HD22	1.64	0.63
1:A:1948:LEU:HD22	1:A:1953:ALA:HB3	1.80	0.63
1:A:2834:GLN:HA	1:A:2837:LEU:HD23	1.80	0.62
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.82	0.62
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.81	0.61
1:A:2838:VAL:HG13	1:A:2839:GLU:HG2	1.83	0.60
1:A:2962:LYS:HE2	1:A:3665:GLY:H	1.67	0.60
1:A:3649:LEU:HD11	1:A:3696:VAL:HG12	1.83	0.60
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.02	0.60
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.83	0.59
1:A:3647:PRO:HG3	1:A:3664:LEU:HB2	1.85	0.59
1:A:4511:LEU:HA	1:A:4514:LEU:HD12	1.85	0.59
1:A:2518:ILE:O	1:A:2522:THR:HB	2.02	0.59
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	1.84	0.59
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.84	0.58
1:A:2154:ILE:HG13	1:A:2155:PRO:HD3	1.85	0.58
1:A:3012:LEU:HD21	1:A:3064:VAL:HG11	1.85	0.58
1:A:2148:LYS:HG3	1:A:2361:MET:HB2	1.84	0.58
1:A:4068:SER:HA	1:A:4095:MET:HB2	1.85	0.58
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.87	0.57
1:A:1750:VAL:HG12	1:A:1811:LEU:HD11	1.87	0.56
1:A:3840:LEU:HA	1:A:3859:ILE:HD11	1.87	0.56
1:A:3007:ARG:HB2	1:A:3017:VAL:HG11	1.85	0.56
1:A:2769:LEU:HG	1:A:2773:MET:HE2	1.87	0.56
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.86	0.56
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.88	0.56
1:A:2085:HIS:HB2	1:A:2361:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2677:GLN:HB2	1:A:2680:ILE:HG22	1.87	0.56
1:A:3779:GLU:HG2	1:A:3782:ARG:HH12	1.70	0.56
1:A:4628:THR:HG22	1:A:4629:LYS:H	1.71	0.56
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.88	0.56
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.87	0.55
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.87	0.55
1:A:4544:ASN:HA	1:A:4573:ASN:HD21	1.72	0.55
1:A:2992:PHE:HD2	1:A:3064:VAL:HG13	1.70	0.55
1:A:1766:LEU:HA	1:A:1769:MET:HE2	1.88	0.55
1:A:2138:ILE:HG23	1:A:2161:LEU:HD21	1.89	0.55
1:A:4413:PHE:O	1:A:4417:VAL:HB	2.07	0.55
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.87	0.54
1:A:3645:LEU:O	1:A:3649:LEU:CB	2.52	0.54
1:A:3623:LEU:HD22	1:A:3664:LEU:HD23	1.88	0.54
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.73	0.54
1:A:1711:VAL:HG12	1:A:1853:VAL:HG21	1.89	0.54
1:A:2862:ASP:O	1:A:2866:ALA:HB2	2.08	0.54
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.08	0.53
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.90	0.53
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	1.91	0.53
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.90	0.53
1:A:4268:PHE:HE1	1:A:4637:GLU:HG2	1.73	0.53
1:A:2922:ILE:HG12	1:A:2933:LEU:HD21	1.91	0.53
1:A:2222:MET:HG2	1:A:2364:PHE:HE2	1.74	0.53
1:A:2609:LEU:HD11	1:A:2660:VAL:HG11	1.91	0.53
1:A:1708:GLU:HA	1:A:1711:VAL:HG22	1.91	0.52
1:A:1860:GLN:HG2	1:A:1865:LYS:HA	1.92	0.52
1:A:3835:ILE:HG12	1:A:3870:ARG:HD3	1.91	0.52
1:A:2083:GLN:HE22	1:A:2150:VAL:HG21	1.75	0.52
1:A:3005:LEU:HD21	1:A:3078:ARG:HD3	1.91	0.52
1:A:4113:LEU:HA	1:A:4116:LEU:HD22	1.91	0.52
1:A:2958:VAL:HA	1:A:2991:ALA:HB3	1.92	0.51
1:A:2533:PRO:HB2	1:A:2535:ILE:HG22	1.92	0.51
1:A:2259:ILE:HD11	1:A:2695:THR:HG22	1.92	0.51
1:A:3767:ILE:HA	1:A:3770:LEU:HD12	1.93	0.51
1:A:2399:LYS:HG3	1:A:2400:GLY:H	1.74	0.50
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.94	0.50
1:A:1899:ARG:HH12	1:A:1982:LEU:HD22	1.76	0.50
1:A:2304:ASP:HA	1:A:2344:GLU:HB3	1.93	0.50
1:A:2464:GLN:HG2	1:A:2583:THR:HA	1.94	0.50
1:A:2150:VAL:HG12	1:A:2152:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:ARG:O	1:A:3725:ASP:CB	2.55	0.50
1:A:4409:LEU:HB3	1:A:4504:LEU:HD21	1.93	0.50
1:A:4211:ASP:HB3	1:A:4252:TYR:HE1	1.76	0.50
1:A:1741:TRP:CZ2	1:A:1750:VAL:HG13	2.47	0.50
1:A:4376:TRP:H	1:A:4376:TRP:CD1	2.29	0.50
1:A:4408:PRO:HB3	1:A:4526:GLN:HE21	1.76	0.50
1:A:2281:THR:HG22	1:A:2325:LEU:HD21	1.94	0.49
1:A:2797:ARG:HH12	1:A:3088:ARG:HD2	1.77	0.49
1:A:2933:LEU:HB3	1:A:3065:VAL:HG22	1.94	0.49
1:A:3691:ASP:O	1:A:3695:ARG:HG2	2.13	0.49
1:A:4444:GLN:HG3	1:A:4449:ARG:HB3	1.95	0.49
1:A:2294:GLU:HA	1:A:2297:LYS:HE3	1.95	0.49
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.94	0.49
1:A:2300:TRP:HE1	1:A:2340:ARG:HD2	1.76	0.48
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.77	0.48
1:A:2648:VAL:HB	1:A:2701:VAL:HG12	1.95	0.48
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.96	0.48
1:A:3624:GLU:O	1:A:3628:ARG:CB	2.59	0.48
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.96	0.48
1:A:2298:ARG:HA	1:A:2338:ASN:HB2	1.95	0.48
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.79	0.48
1:A:4052:SER:HB3	1:A:4097:LYS:HE3	1.96	0.48
1:A:1917:LYS:HG2	1:A:1927:VAL:HG11	1.95	0.47
1:A:2553:PRO:HD2	1:A:2570:PRO:HB2	1.96	0.47
1:A:3626:ALA:HA	1:A:3631:ASN:HD21	1.79	0.47
1:A:1975:VAL:HA	1:A:1978:ILE:HG12	1.96	0.47
1:A:1930:PHE:HZ	1:A:1944:ILE:HG21	1.79	0.47
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.96	0.47
1:A:3973:LEU:HD12	1:A:3992:LEU:HD21	1.96	0.47
1:A:2241:LEU:HB3	1:A:2298:ARG:HH22	1.79	0.47
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.96	0.47
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.80	0.47
1:A:3977:GLU:HG2	1:A:3978:THR:HG23	1.96	0.47
1:A:2221:MET:HB2	1:A:2361:MET:HG2	1.97	0.47
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.49	0.47
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.97	0.47
1:A:1813:THR:HG23	1:A:1880:VAL:HG22	1.95	0.47
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	1.96	0.47
1:A:2872:LEU:HD23	1:A:2920:LEU:HD12	1.97	0.47
1:A:4065:GLN:HB3	1:A:4092:ARG:HD2	1.96	0.47
1:A:2231:SER:HB3	1:A:2344:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.79	0.46
1:A:4544:ASN:HD22	1:A:4591:ARG:HH22	1.62	0.46
1:A:2979:VAL:HG13	1:A:2990:ILE:HD13	1.98	0.46
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.79	0.46
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.97	0.46
1:A:3624:GLU:HA	1:A:3669:ILE:HG22	1.97	0.46
1:A:1713:LEU:HA	1:A:1716:LEU:HG	1.98	0.46
1:A:2519:ARG:HE	1:A:2534:ILE:HD11	1.80	0.46
1:A:2620:LEU:HD11	1:A:2630:LEU:HD21	1.98	0.46
1:A:2775:GLU:HA	1:A:2778:THR:HG22	1.96	0.46
1:A:3730:ASP:HA	1:A:3733:LYS:HD2	1.98	0.46
1:A:4413:PHE:CZ	1:A:4417:VAL:HG21	2.51	0.46
1:A:1814:GLU:O	1:A:1818:GLN:HG2	2.16	0.46
1:A:2581:LEU:O	1:A:2585:LEU:HB2	2.17	0.45
1:A:3874:GLY:HA3	1:A:4144:ILE:HG23	1.97	0.45
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	1.99	0.45
1:A:4288:VAL:HG21	1:A:4294:ILE:HG13	1.97	0.45
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.98	0.45
1:A:3642:ASP:HB3	1:A:3645:LEU:HG	1.99	0.45
1:A:4179:LEU:HD12	1:A:4223:LEU:HD11	1.98	0.45
1:A:1964:GLU:H	1:A:1967:MET:HE3	1.81	0.45
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.52	0.45
1:A:4211:ASP:HB3	1:A:4252:TYR:CE1	2.51	0.45
1:A:3703:VAL:HG11	1:A:3829:LEU:HD22	1.97	0.44
1:A:2075:LEU:HG	1:A:2160:LEU:HD13	1.97	0.44
1:A:2446:ILE:HG22	1:A:2505:ASP:HB2	1.99	0.44
1:A:2935:LEU:HD23	1:A:3092:ASN:HB2	2.00	0.44
1:A:3614:PHE:HE2	1:A:3640:SER:HB2	1.82	0.44
1:A:4066:ILE:HD11	1:A:4095:MET:HG2	2.00	0.44
1:A:4502:LYS:HE2	1:A:4502:LYS:HB2	1.83	0.44
1:A:1985:HIS:CE1	1:A:1992:LYS:HD2	2.52	0.44
1:A:2684:ARG:HD2	1:A:2726:ARG:HB3	1.99	0.44
1:A:2252:HIS:HB2	1:A:2301:ILE:HG12	1.99	0.44
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.52	0.44
1:A:3724:VAL:HA	1:A:3727:LYS:HB2	1.97	0.44
1:A:1729:LYS:HA	1:A:1729:LYS:HD3	1.67	0.44
1:A:2228:SER:HB2	1:A:2364:PHE:HB3	2.00	0.44
1:A:2368:VAL:HG12	1:A:2369:LEU:HD12	2.00	0.44
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	2.00	0.44
1:A:1751:VAL:HG11	1:A:1878:LYS:HE3	1.99	0.44
1:A:4504:LEU:HA	1:A:4507:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2513:GLU:O	1:A:2516:GLU:HG3	2.18	0.44
1:A:4395:LEU:HD22	1:A:4424:LEU:HD12	2.00	0.44
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.98	0.43
1:A:4158:LEU:HD21	1:A:4310:GLU:HG2	1.99	0.43
1:A:1687:LYS:HE3	1:A:1715:LYS:HD2	2.00	0.43
1:A:2104:LYS:HB2	1:A:2136:ILE:HG21	2.01	0.43
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.00	0.43
1:A:1891:THR:HG21	1:A:2039:LEU:HD11	2.00	0.43
1:A:1899:ARG:HH21	1:A:1985:HIS:HB3	1.84	0.43
1:A:3600:ILE:HD13	1:A:3634:LEU:HD13	2.01	0.43
1:A:1800:GLN:H	1:A:1805:ARG:HH22	1.67	0.43
1:A:2996:GLU:HB3	1:A:3068:MET:HB3	2.01	0.43
1:A:3487:GLU:O	1:A:3490:GLU:HG3	2.19	0.43
1:A:3627:LEU:HD23	1:A:3669:ILE:HD12	2.00	0.43
1:A:4408:PRO:HB2	1:A:4523:ALA:HB1	2.00	0.43
1:A:1891:THR:HG22	1:A:4250:SER:HA	2.01	0.42
1:A:3031:THR:HA	1:A:3034:LYS:HG2	2.01	0.42
1:A:2278:GLY:O	1:A:2282:HIS:CB	2.67	0.42
1:A:3513:PHE:HZ	1:A:3575:GLU:HG2	1.84	0.42
1:A:3818:LEU:HA	1:A:4346:MET:HE1	2.01	0.42
1:A:3846:LEU:HD11	1:A:3859:ILE:HD13	2.00	0.42
1:A:2440:ALA:HA	1:A:2443:LEU:HD13	2.00	0.42
1:A:3154:LEU:HD22	1:A:3516:TYR:CD2	2.55	0.42
1:A:2862:ASP:O	1:A:2866:ALA:CB	2.67	0.42
1:A:3588:LEU:HD21	1:A:3688:PHE:CZ	2.54	0.42
1:A:3945:LYS:HA	1:A:3945:LYS:HD3	1.81	0.42
1:A:4246:LEU:HA	1:A:4246:LEU:HD23	1.82	0.42
1:A:2593:LEU:HD11	1:A:2605:LEU:HD13	2.02	0.42
1:A:2838:VAL:HG23	1:A:3093:TRP:CZ2	2.55	0.42
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.34	0.42
1:A:1742:ILE:HG23	1:A:1807:LYS:HD2	2.02	0.42
1:A:2065:LEU:HD12	1:A:2137:LEU:HD22	2.00	0.42
1:A:2755:MET:HG3	1:A:2807:PHE:HD1	1.85	0.42
1:A:2222:MET:HG2	1:A:2364:PHE:CE2	2.55	0.42
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	2.01	0.42
1:A:2440:ALA:HB3	1:A:2502:LEU:HD12	2.02	0.42
1:A:2615:MET:HE2	1:A:2615:MET:HB2	1.99	0.42
1:A:3123:PRO:HG2	1:A:3126:MET:HB2	2.02	0.42
1:A:4631:ASP:HB3	1:A:4634:SER:H	1.85	0.42
1:A:2277:ASP:HB3	1:A:2282:HIS:HB2	2.02	0.42
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4431:LEU:HD12	1:A:4431:LEU:HA	1.89	0.42
1:A:4541:LEU:HD11	1:A:4590:LEU:HD22	2.02	0.42
1:A:2413:LEU:HD23	1:A:2416:GLN:HE21	1.83	0.41
1:A:2072:PHE:HB2	1:A:2164:VAL:HG11	2.02	0.41
1:A:3157:ALA:HA	1:A:3160:ARG:HE	1.84	0.41
1:A:4038:ASN:HB3	1:A:4118:PRO:HG3	2.01	0.41
1:A:3070:PRO:HB3	1:A:3093:TRP:HH2	1.86	0.41
1:A:4408:PRO:HG3	1:A:4527:TYR:HB2	2.03	0.41
1:A:1914:GLU:HG3	3:A:4701:ADP:H3'	2.02	0.41
1:A:2156:LEU:HD11	1:A:4411:ARG:HD3	2.01	0.41
1:A:2993:ILE:HD13	1:A:3065:VAL:HB	2.02	0.41
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.56	0.41
1:A:3662:ILE:H	1:A:3669:ILE:HD11	1.85	0.41
1:A:3819:LYS:HE3	1:A:3819:LYS:HB2	1.88	0.41
1:A:3907:HIS:CG	1:A:3941:LEU:HD11	2.55	0.41
1:A:3597:THR:HA	1:A:3600:ILE:HG22	2.02	0.41
1:A:3740:LEU:HA	1:A:3743:ARG:HG2	2.01	0.41
1:A:4565:LEU:HD12	1:A:4642:VAL:HG22	2.02	0.41
1:A:2175:MET:HE2	1:A:2175:MET:HB3	1.92	0.41
1:A:2181:GLU:HG3	1:A:2244:LEU:HD13	2.01	0.41
1:A:2854:ALA:O	1:A:2858:PHE:HB2	2.21	0.41
1:A:3021:PHE:HB3	1:A:3029:LEU:HD21	2.02	0.41
1:A:3136:PRO:HA	1:A:3137:PRO:HD3	1.92	0.41
1:A:4189:ILE:HD12	1:A:4321:LEU:HA	2.02	0.41
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.03	0.40
1:A:4268:PHE:CE1	1:A:4637:GLU:HG2	2.55	0.40
1:A:2443:LEU:HD23	1:A:2510:MET:HB3	2.02	0.40
1:A:2532:ILE:HD12	1:A:2533:PRO:HD2	2.03	0.40
1:A:2684:ARG:HA	1:A:2687:VAL:HG12	2.03	0.40
1:A:2822:ILE:HD11	1:A:2866:ALA:HB1	2.03	0.40
1:A:4489:LEU:HA	1:A:4492:ILE:HG22	2.04	0.40
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.02	0.40
1:A:2050:ALA:HB2	1:A:2093:LEU:HD21	2.03	0.40
1:A:4492:ILE:HD13	1:A:4507:ILE:HG21	2.02	0.40
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.86	0.40
1:A:3134:PRO:HD2	1:A:3141:GLU:HG2	2.03	0.40
1:A:2661:LEU:HD23	1:A:2661:LEU:HA	1.92	0.40
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ATP	A	4704	-	32,33,33	0.34	0	48,52,52	0.35	0
3	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
4	ATP	A	4702	5	32,33,33	0.39	0	48,52,52	0.33	0
3	ADP	A	4705	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	4704	-	-	6/22/38/38	0/3/3/3
3	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
4	ATP	A	4702	5	-	2/22/38/38	0/3/3/3
3	ADP	A	4705	-	-	3/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4701	ADP	C5-C4	4.65	1.47	1.39
3	A	4705	ADP	C5-C4	4.59	1.47	1.39
3	A	4705	ADP	C5-C6	2.67	1.48	1.41
3	A	4701	ADP	C5-C6	2.57	1.48	1.41
3	A	4701	ADP	C5-N7	-2.40	1.34	1.39
3	A	4705	ADP	C8-N7	2.36	1.36	1.31
3	A	4705	ADP	C5-N7	-2.31	1.34	1.39
3	A	4701	ADP	C8-N7	2.26	1.36	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4701	ADP	C5-C4-N3	-5.86	118.64	126.72
3	A	4705	ADP	C5-C4-N3	-5.71	118.86	126.72
3	A	4701	ADP	N3-C4-N9	4.74	135.24	127.17
3	A	4705	ADP	N3-C4-N9	4.43	134.70	127.17
3	A	4701	ADP	C2-N3-C4	3.74	120.96	111.83
3	A	4705	ADP	C2-N3-C4	3.62	120.66	111.83
3	A	4705	ADP	C4-C5-N7	-3.60	106.46	110.58
3	A	4701	ADP	N3-C2-N1	-3.39	123.45	128.58
3	A	4701	ADP	C4-C5-N7	-3.24	106.87	110.58
3	A	4705	ADP	N3-C2-N1	-3.17	123.79	128.58
3	A	4705	ADP	C4-N9-C8	2.67	108.54	105.74
3	A	4705	ADP	C5-N7-C8	2.60	107.54	103.45
3	A	4701	ADP	C4-N9-C8	2.52	108.38	105.74
3	A	4701	ADP	C5-N7-C8	2.35	107.15	103.45
3	A	4701	ADP	C3'-C2'-C1'	2.18	105.59	101.46
3	A	4705	ADP	C6-C5-N7	2.14	136.21	132.09
3	A	4705	ADP	C3'-C2'-C1'	2.07	105.37	101.46
3	A	4705	ADP	N9-C8-N7	-2.06	111.01	113.94
3	A	4705	ADP	O4'-C1'-N9	2.03	112.00	108.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

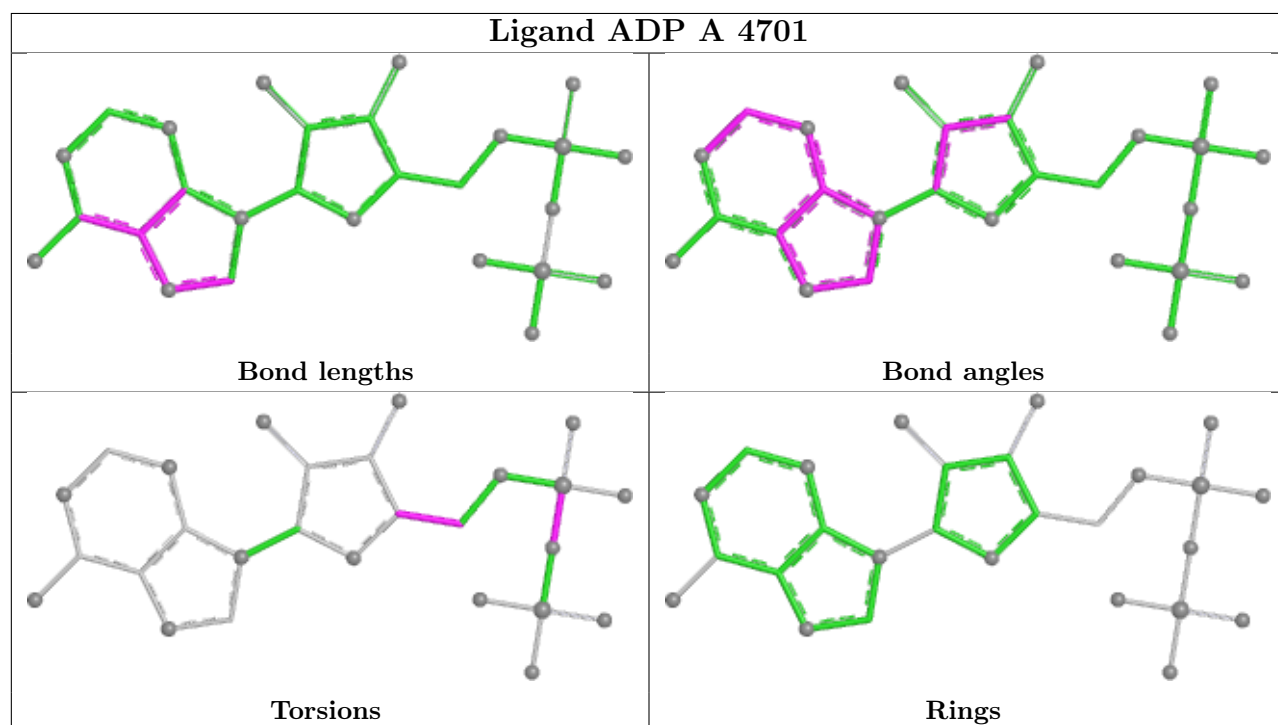
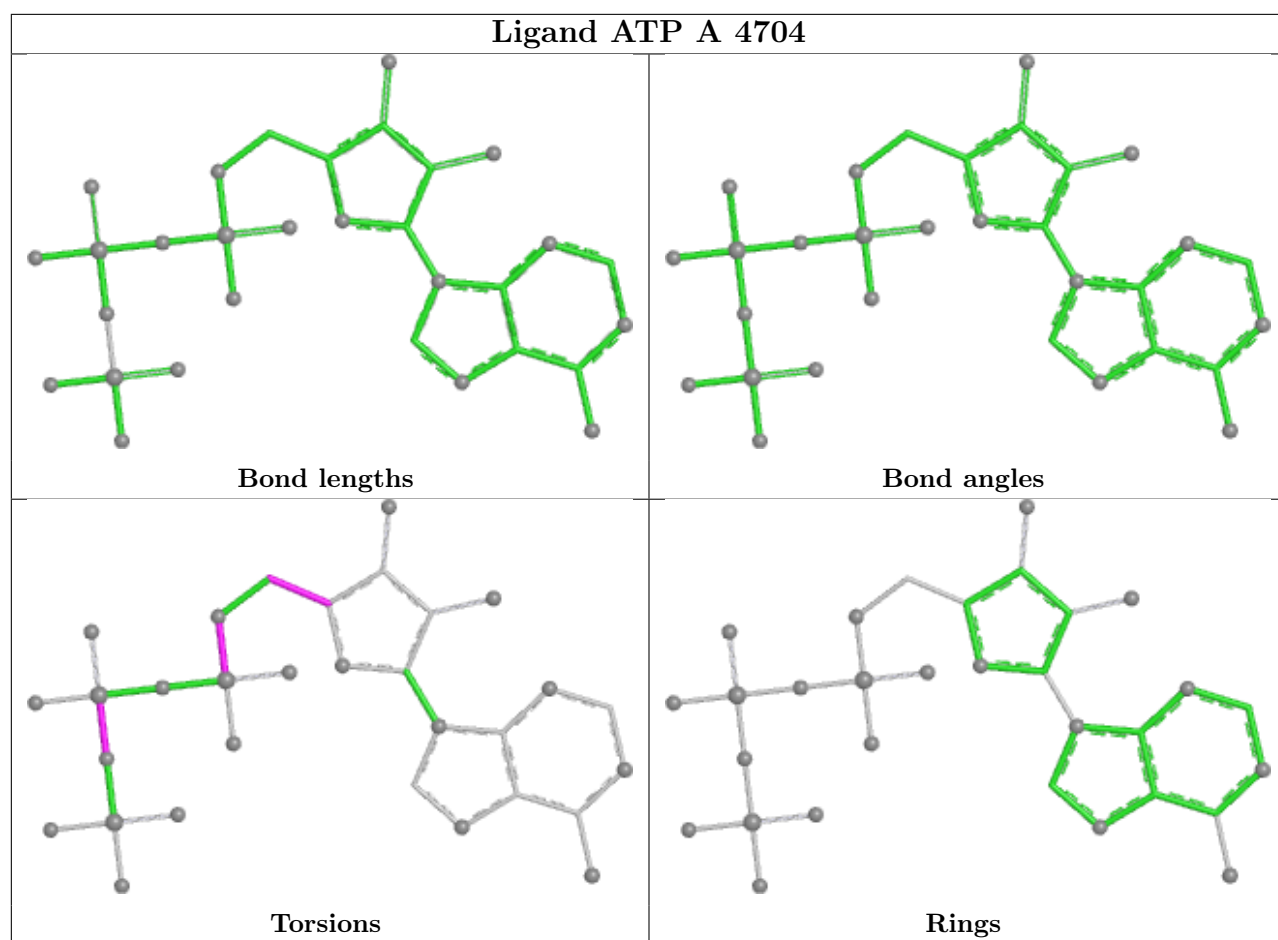
Mol	Chain	Res	Type	Atoms
3	A	4705	ADP	C5'-O5'-PA-O1A
3	A	4705	ADP	C5'-O5'-PA-O2A
3	A	4705	ADP	C5'-O5'-PA-O3A
4	A	4704	ATP	C5'-O5'-PA-O1A
4	A	4704	ATP	C5'-O5'-PA-O3A
4	A	4704	ATP	O4'-C4'-C5'-O5'
4	A	4704	ATP	C3'-C4'-C5'-O5'
3	A	4701	ADP	PB-O3A-PA-O1A
4	A	4702	ATP	PG-O3B-PB-O1B
4	A	4704	ATP	C5'-O5'-PA-O2A
3	A	4701	ADP	PB-O3A-PA-O2A
3	A	4701	ADP	O4'-C4'-C5'-O5'
4	A	4704	ATP	PG-O3B-PB-O2B
4	A	4702	ATP	PG-O3B-PB-O2B

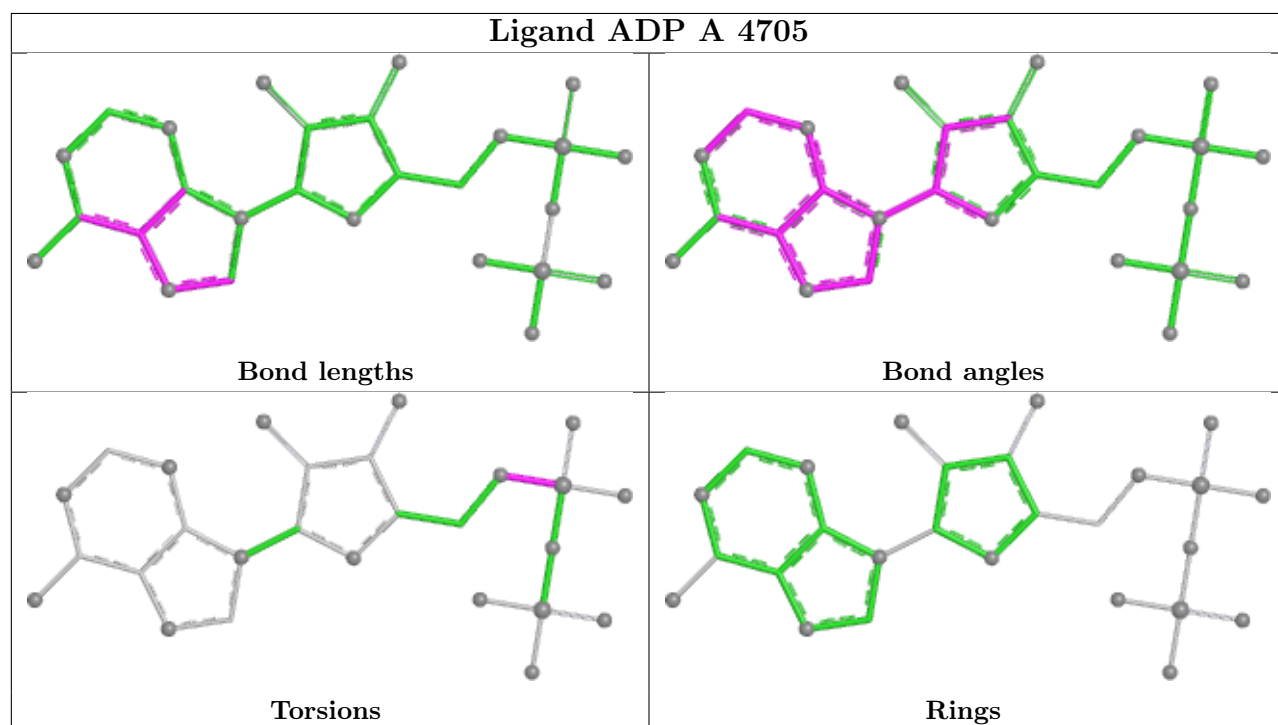
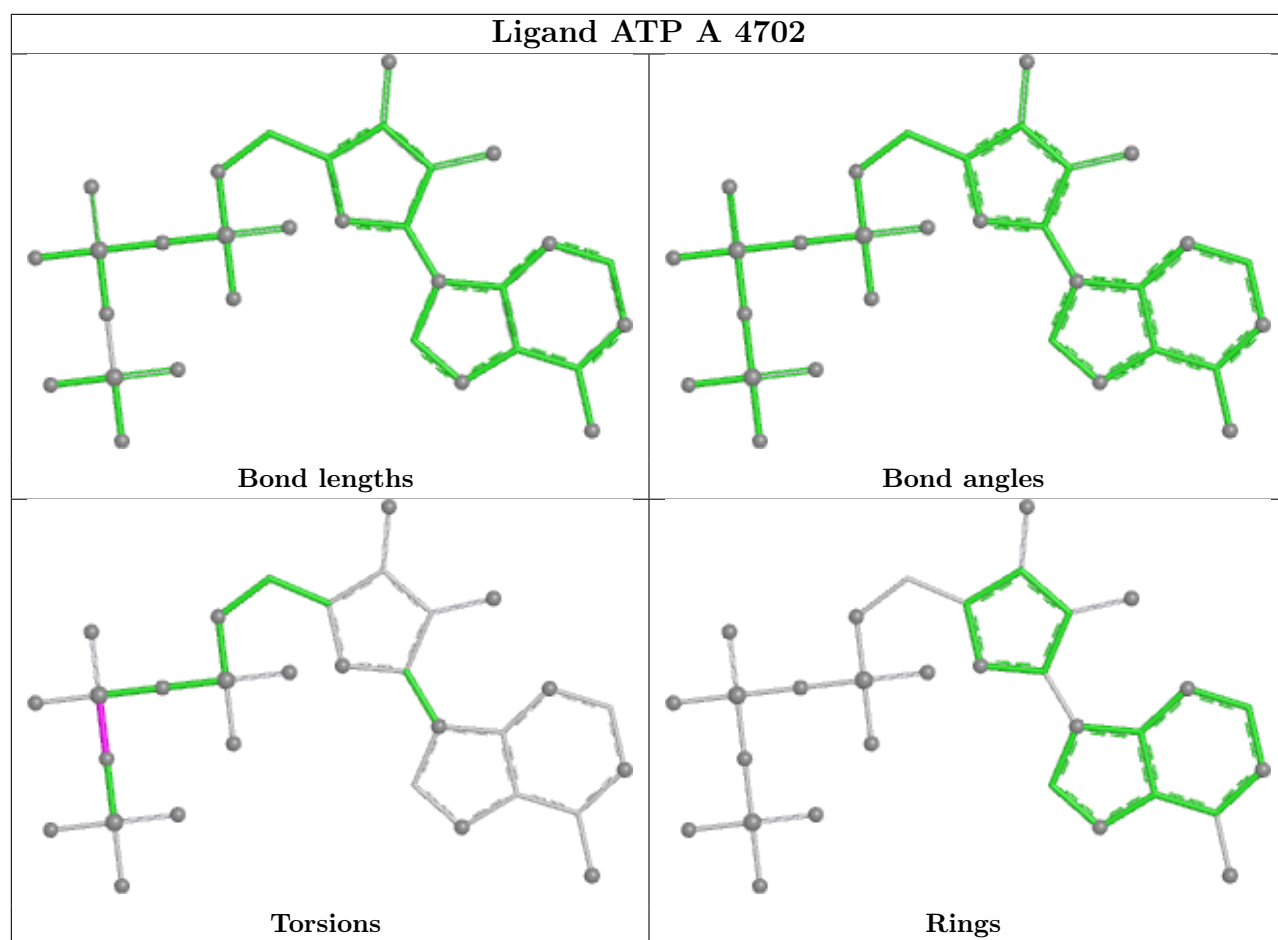
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4701	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

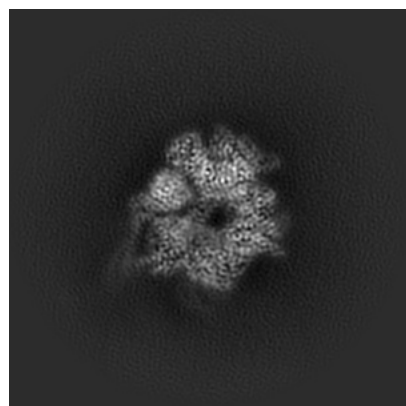
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47429. These allow visual inspection of the internal detail of the map and identification of artifacts.

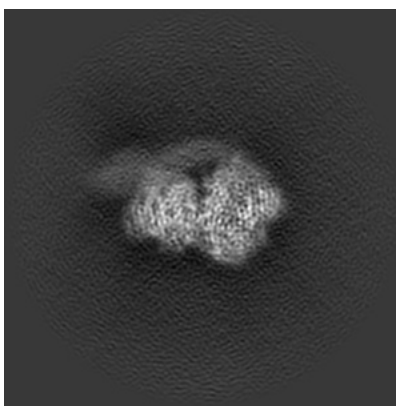
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

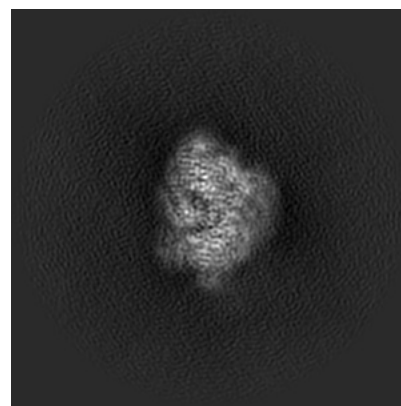
#### 6.1.1 Primary map



X

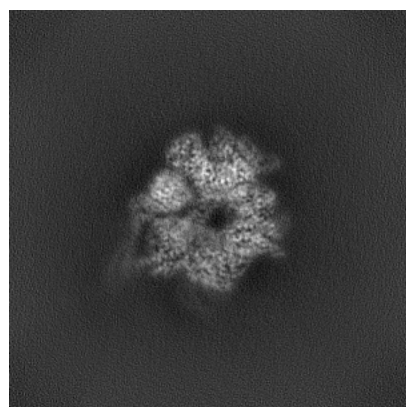


Y

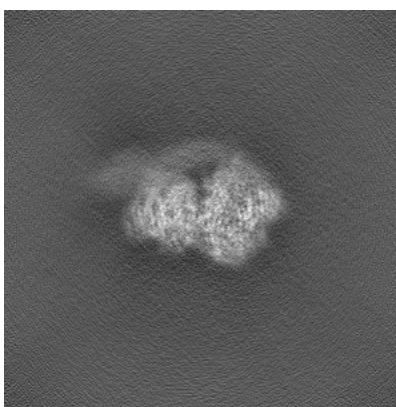


Z

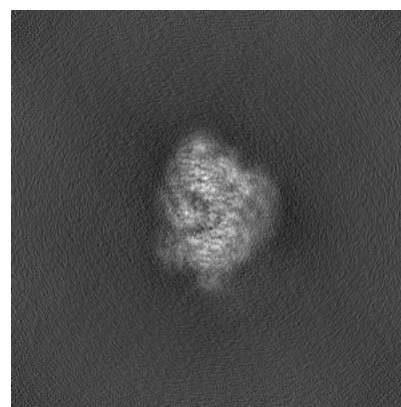
#### 6.1.2 Raw map



X



Y

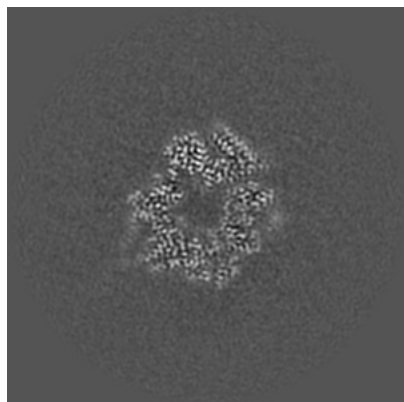


Z

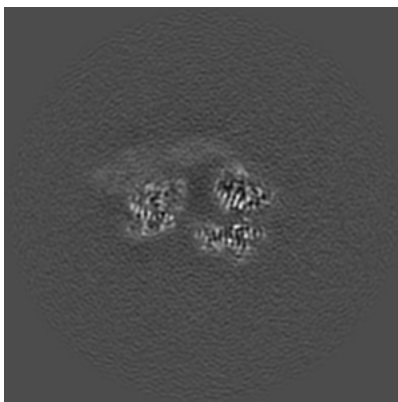
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

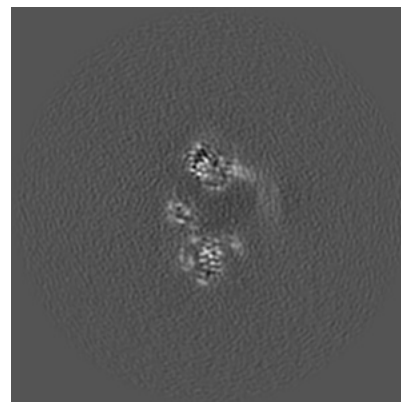
### 6.2.1 Primary map



X Index: 176

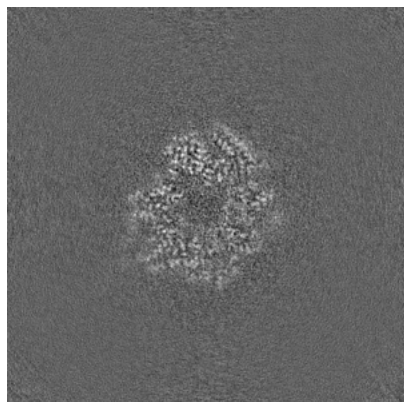


Y Index: 176

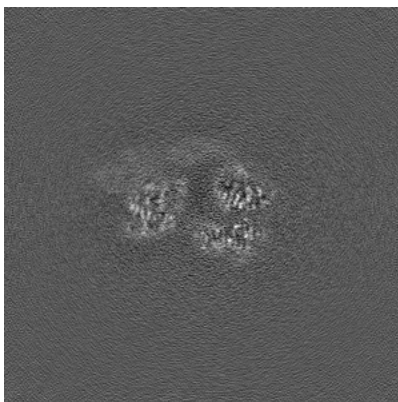


Z Index: 176

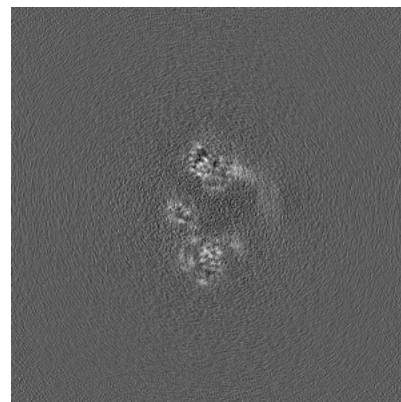
### 6.2.2 Raw map



X Index: 176



Y Index: 176



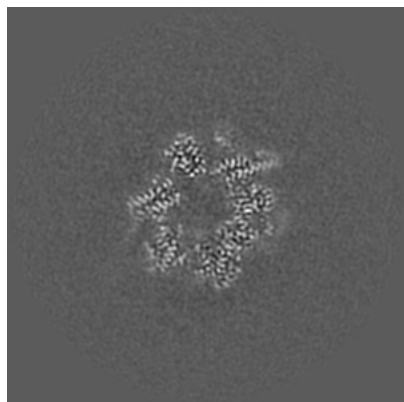
Z Index: 176

The images above show central slices of the map in three orthogonal directions.

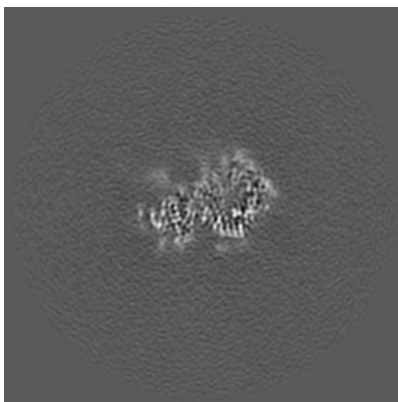


## 6.3 Largest variance slices [i](#)

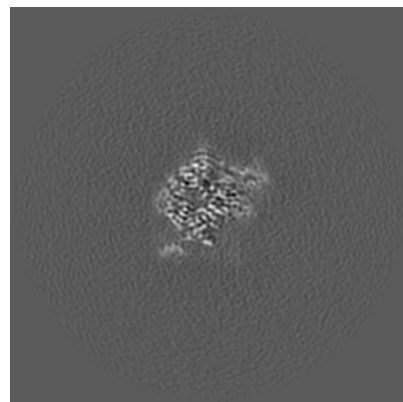
### 6.3.1 Primary map



X Index: 170

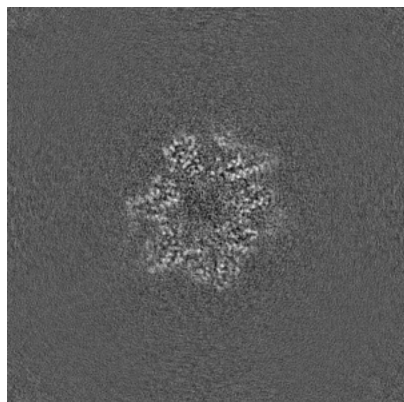


Y Index: 204

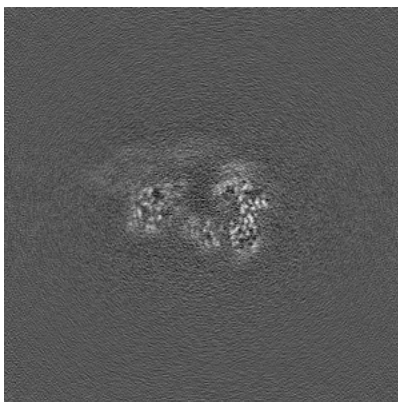


Z Index: 208

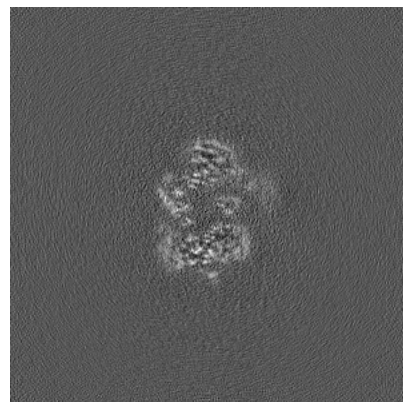
### 6.3.2 Raw map



X Index: 172



Y Index: 171

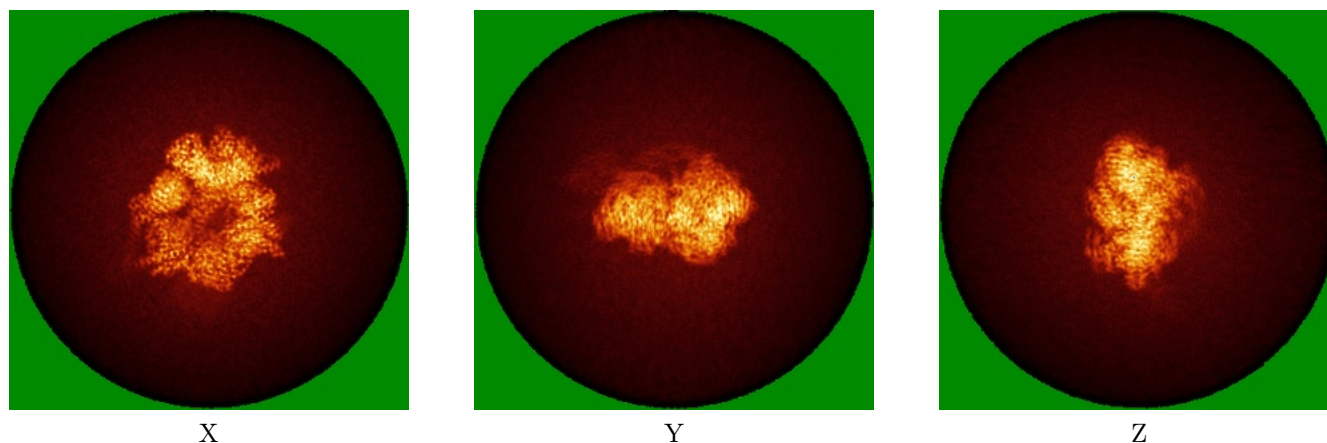


Z Index: 188

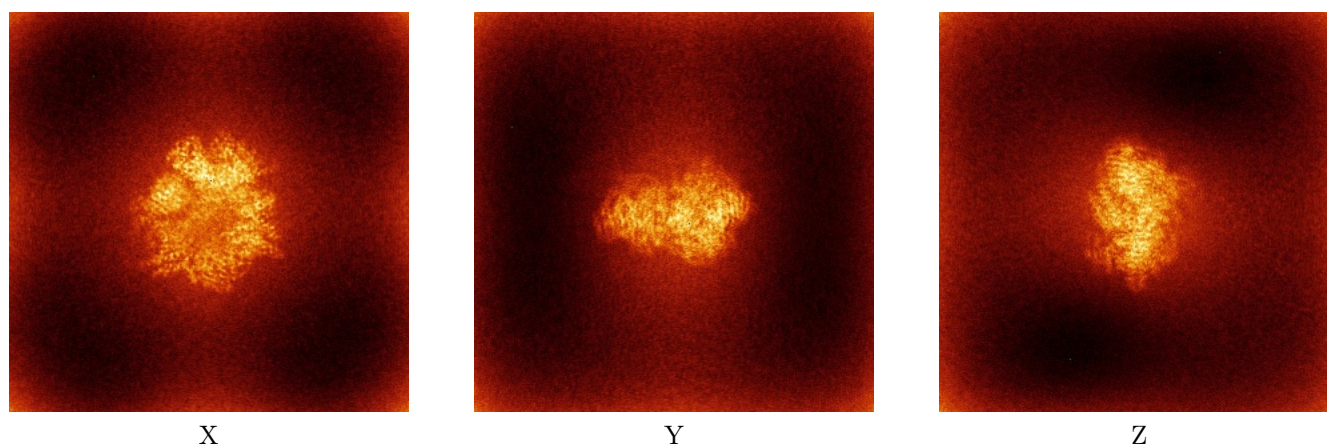
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

This section was not generated.

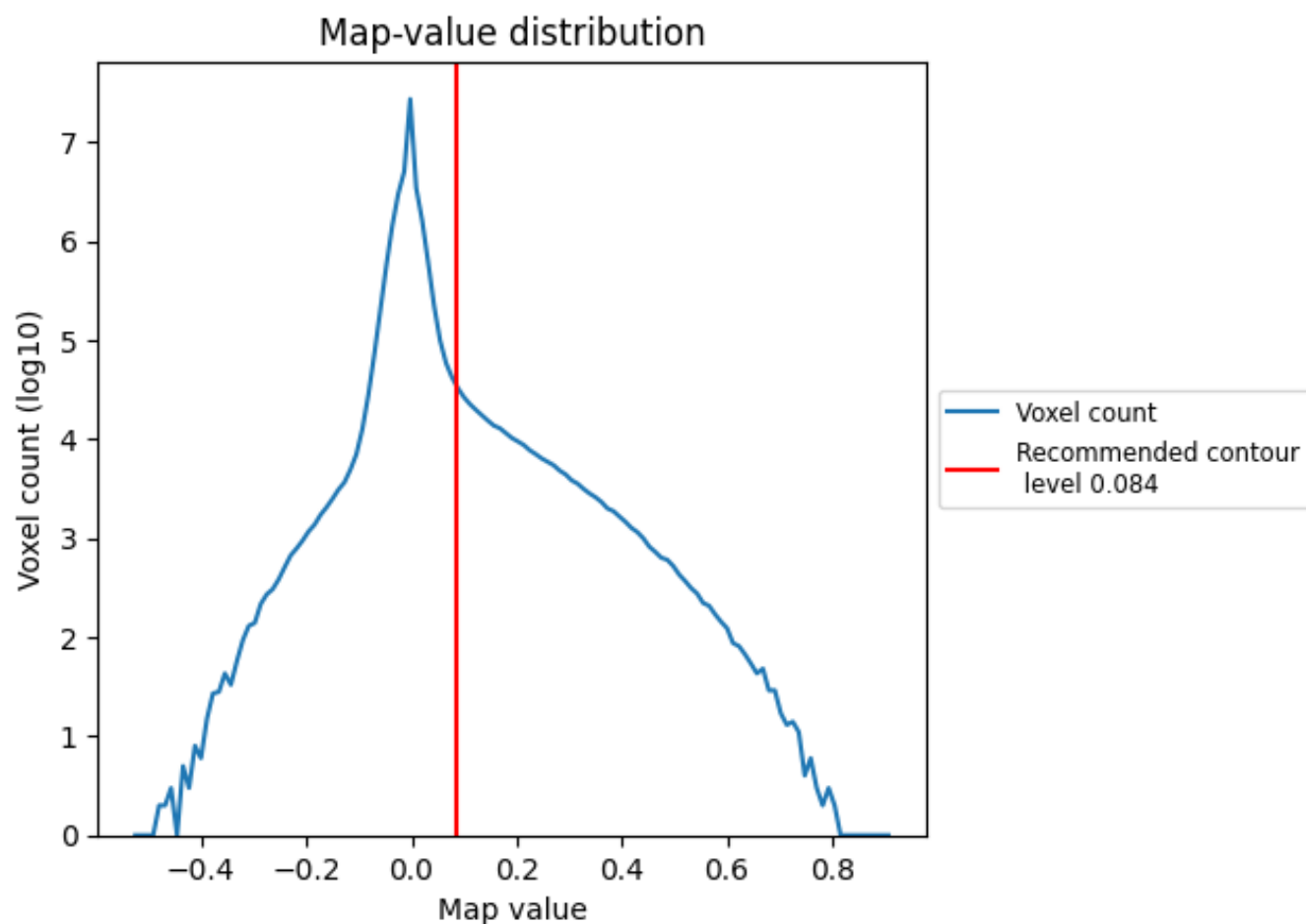
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

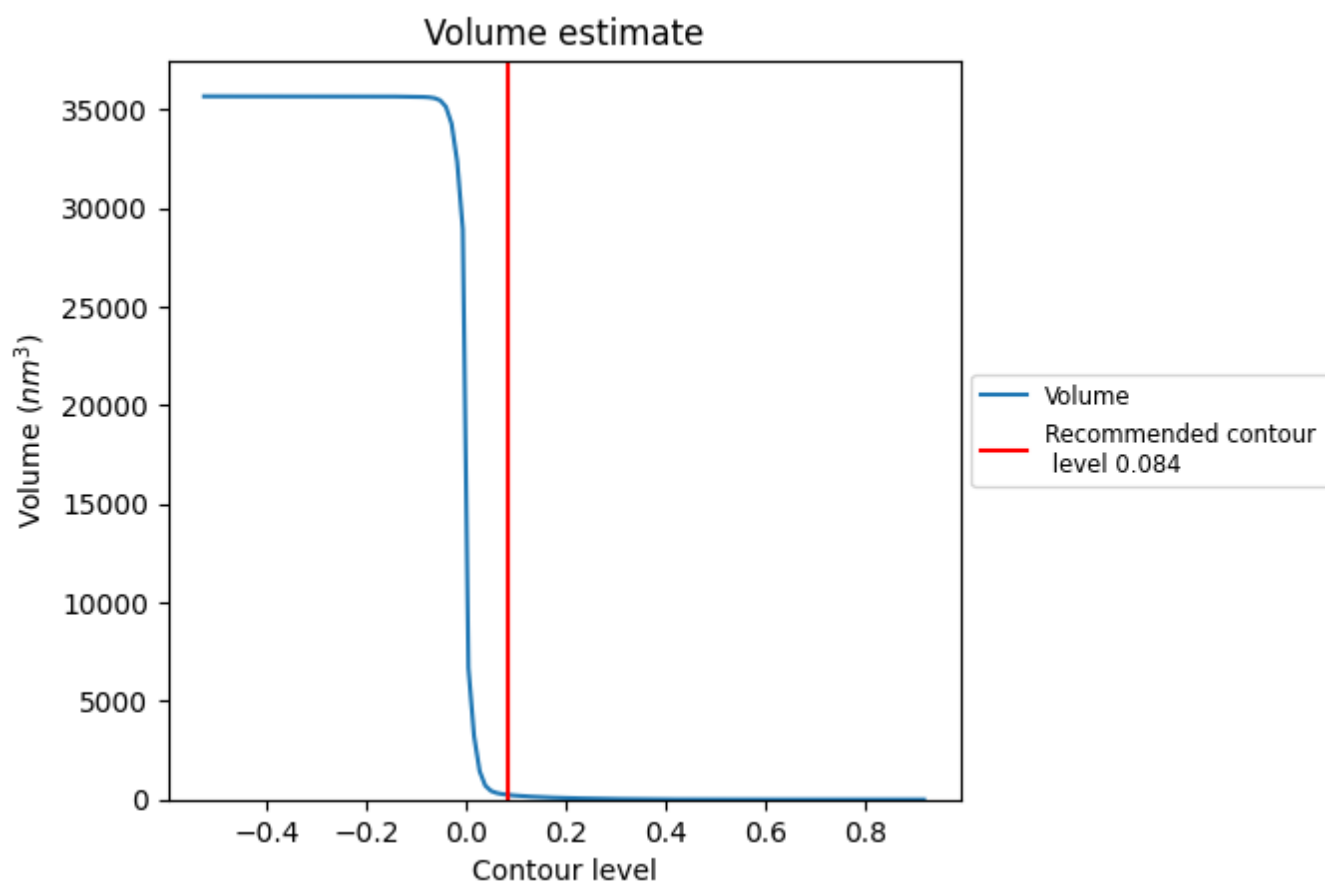
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

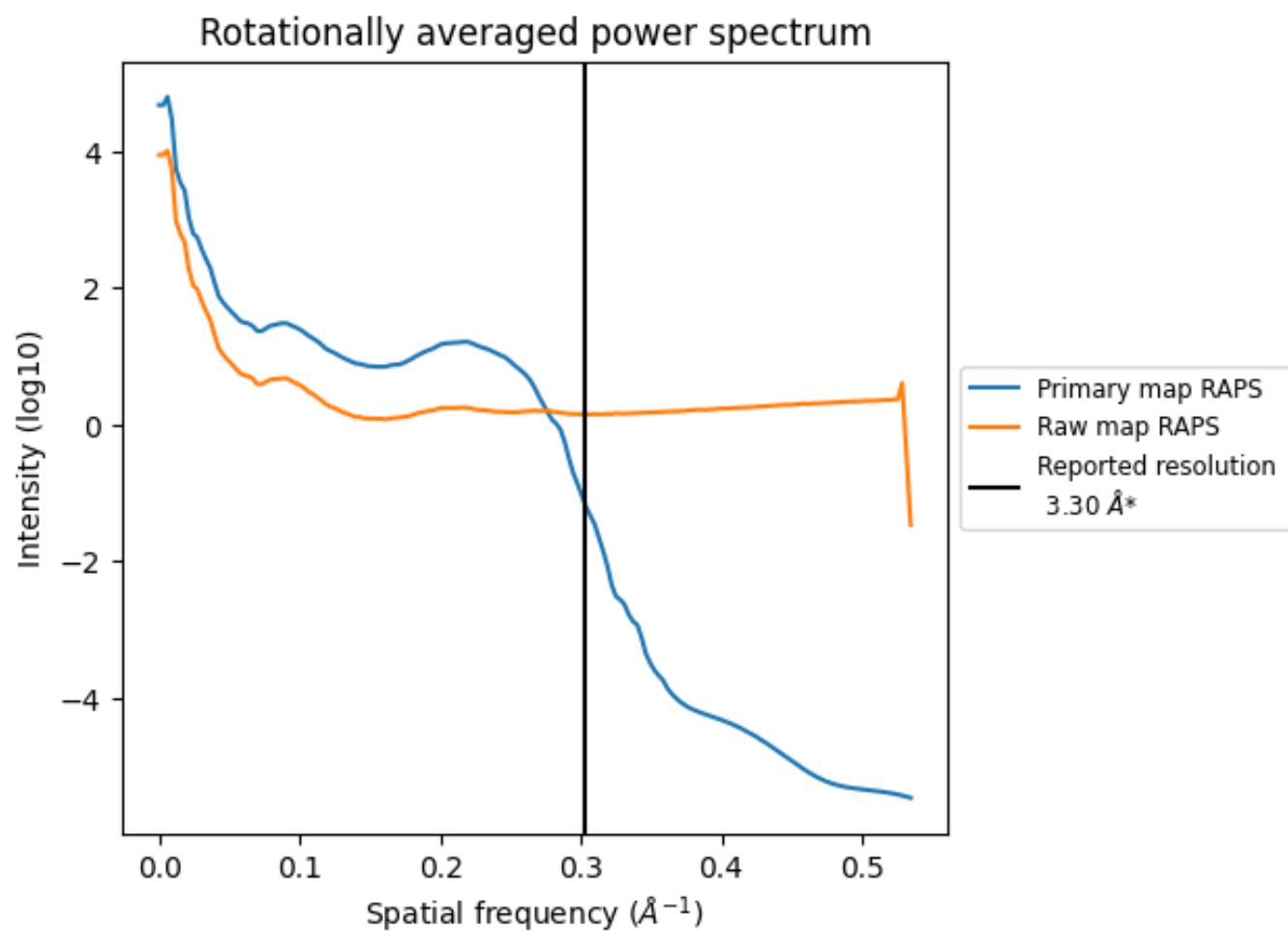
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm<sup>3</sup>; this corresponds to an approximate mass of 215 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

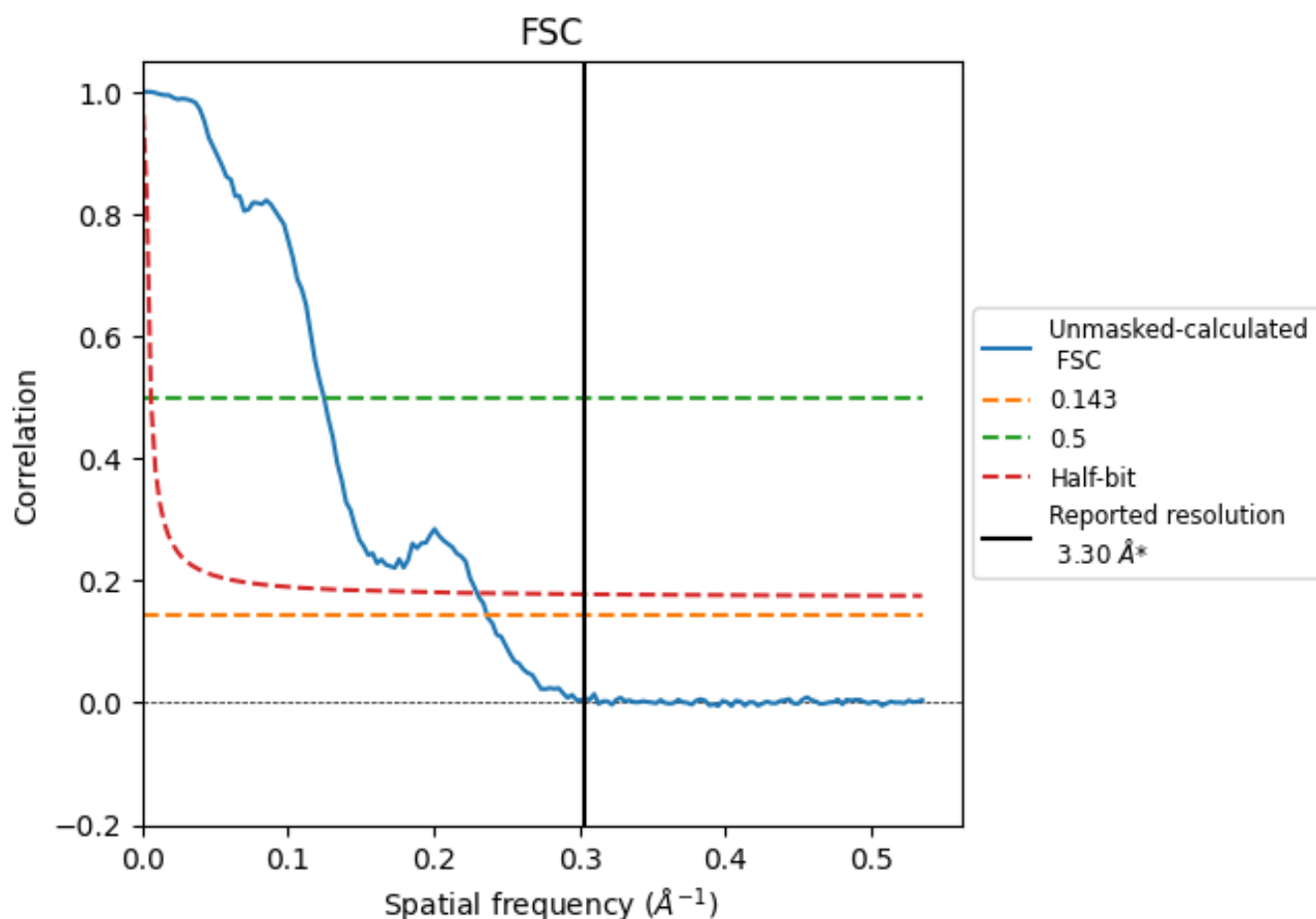


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	8.03	4.36

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.23 differs from the reported value 3.3 by more than 10 %



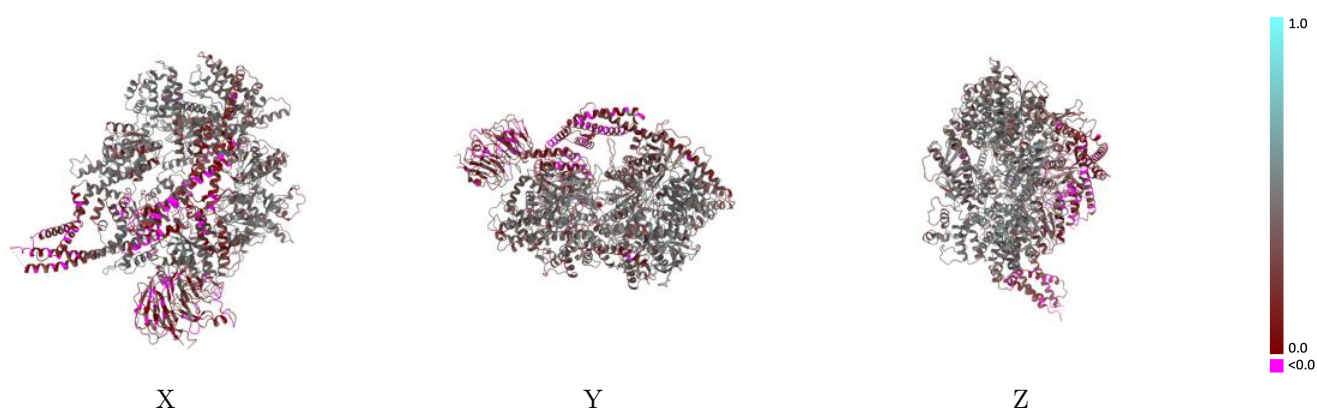
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47429 and PDB model 9E22. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)

This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)

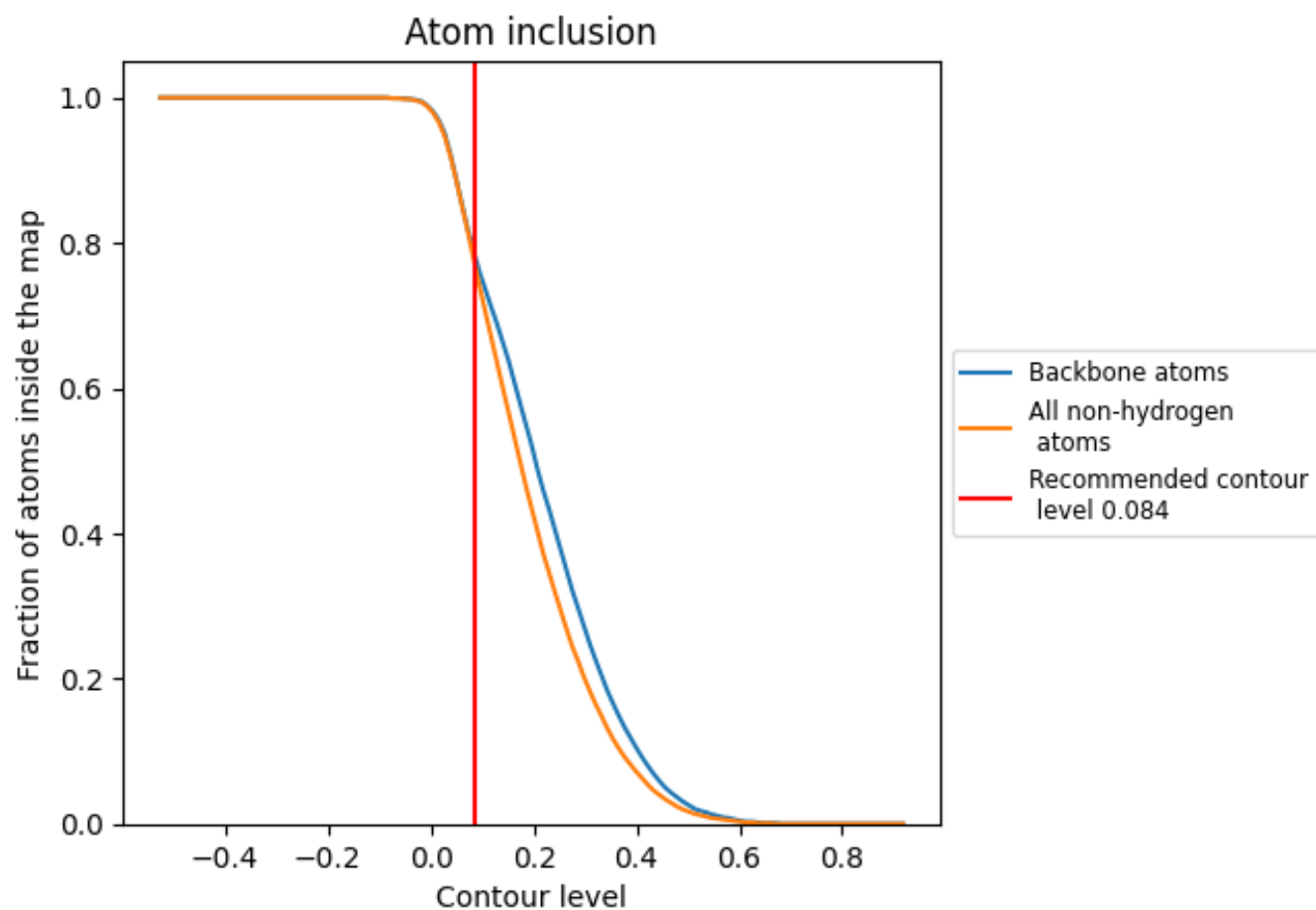


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7760	<div></div> 0.3650
A	<div></div> 0.8210	<div></div> 0.3770
E	<div></div> 0.1320	<div></div> 0.1830

